Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:57 AM GMT

PDB ID	:	3QJQ
Title	:	The structure of and photolytic induced changes of carbon monoxide binding to the cytochrome ba3-oxidase from Thermus thermophilus
Authors	:	Liu, B.; Zhang, Y.; Sage, J.T.; Doukov, T.; Chen, Y.; Stout, C.D.; Fee, J.A
Deposited on	:	2011-01-30
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

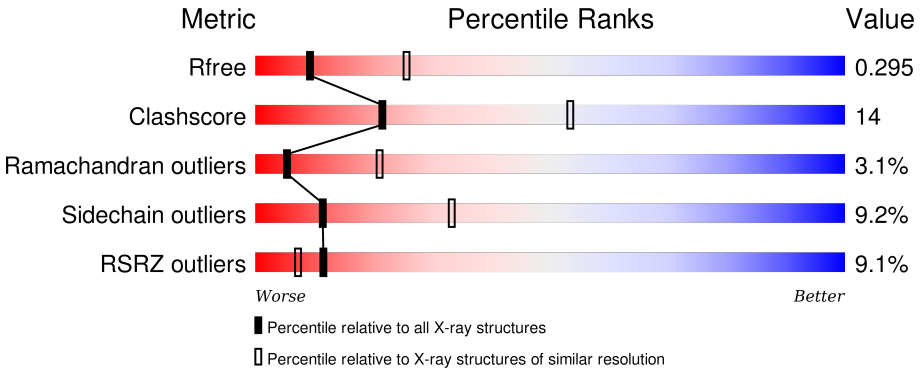
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	568	8% 65% 28%
2	B	168	11% 63% 32%
3	C	34	12% 44% 35% 18%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6037 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4367	2962	699	690	16			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	EXPRESSION TAG	UNP Q5SJ79
A	-4	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	-3	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	-2	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	-1	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	0	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	1	HIS	-	EXPRESSION TAG	UNP Q5SJ79

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	166	Total	C	N	O	S	0	0	0
			1298	844	216	234	4			

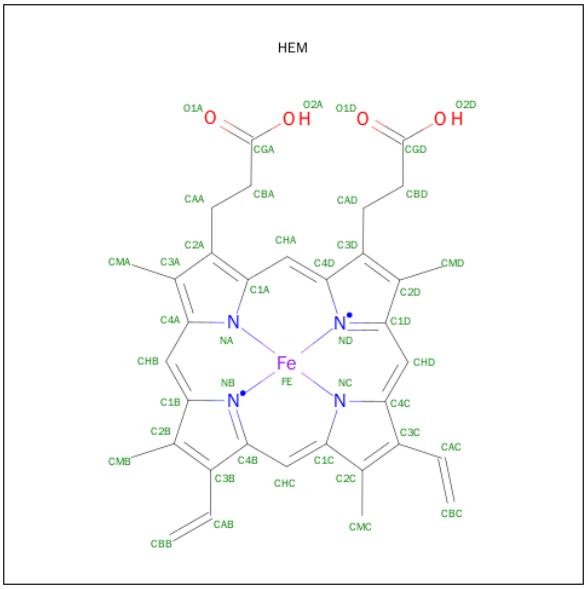
- Molecule 3 is a protein called Cytochrome c oxidase polypeptide 2A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	33	Total	C	N	O	0	0	0
			259	179	39	41			

- Molecule 4 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

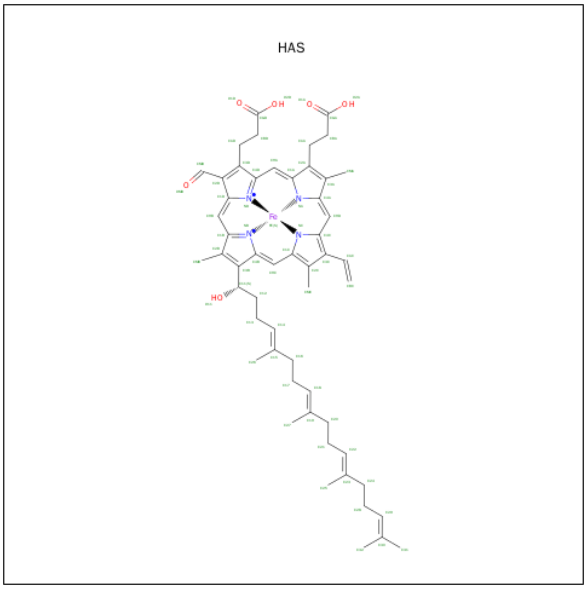
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cu	0	0
			1	1		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



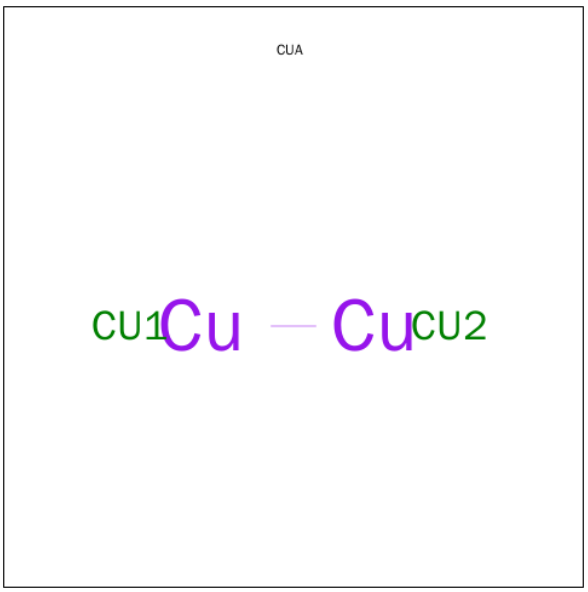
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is HEME-AS (three-letter code: HAS) (formula: $C_{54}H_{64}FeN_4O_6$).



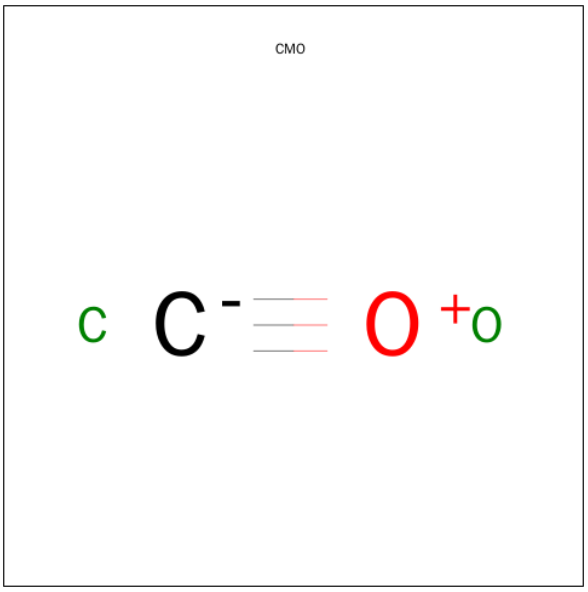
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Fe	N	O	0	0
			65	54	1	4	6		

- Molecule 7 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Cu 2 2	0	0

- Molecule 8 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



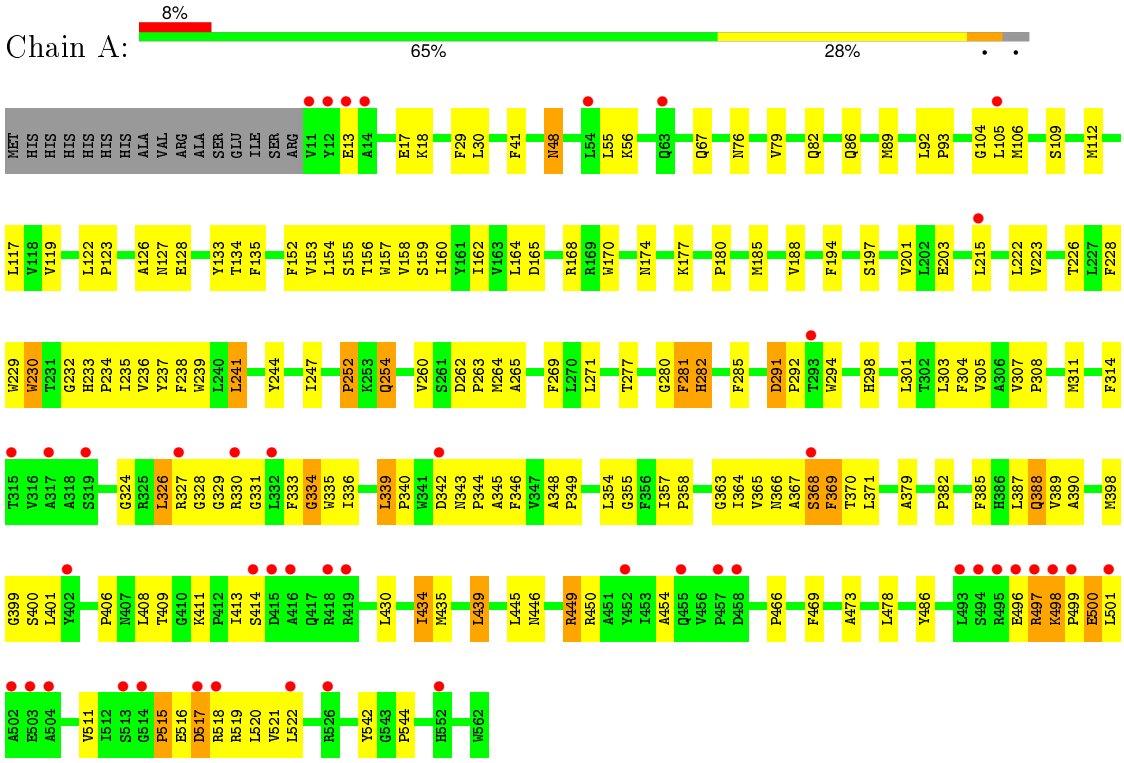
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 2 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

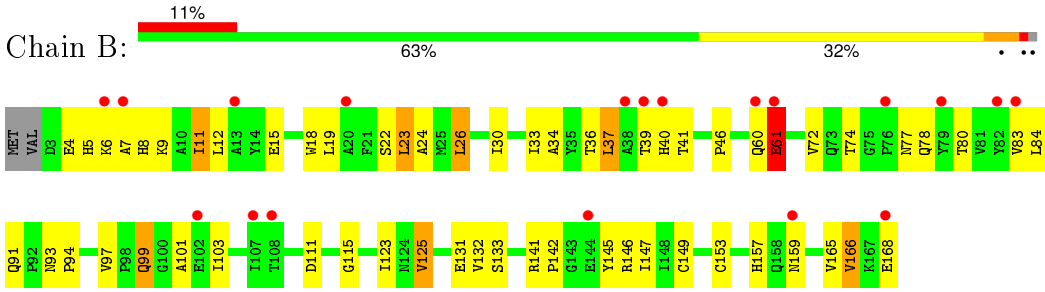
- Molecule 1: Cytochrome c oxidase subunit 1

Chain A:



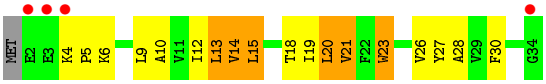
- Molecule 2: Cytochrome c oxidase subunit 2

Chain B:



- Molecule 3: Cytochrome c oxidase polypeptide 2A

Chain C:


MET1
E2
E3
K4
P5
K6
L9
A10
V11
I12
L13
V14
L15
T18
I19
L20
V21
F22
W23
V26
Y27
A28
V29
F30
G34

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	108.77Å 108.77Å 164.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.88 – 2.90 19.88 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.88-2.90) 99.5 (19.88-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.02	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.229 , 0.284 0.240 , 0.295	Depositor DCC
R_{free} test set	1144 reflections (5.39%)	DCC
Wilson B-factor (Å^2)	90.5	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 75.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 22380 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6037	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CMO, HEM, HAS, CUA, CU1

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.64	0/4524	0.76	0/6210
2	B	0.63	1/1335 (0.1%)	0.74	2/1822 (0.1%)
3	C	0.86	0/265	0.89	0/359
All	All	0.65	1/6124 (0.0%)	0.76	2/8391 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	153	CYS	CB-SG	-6.01	1.72	1.82

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	26	LEU	CB-CG-CD2	-9.56	94.75	111.00
2	B	26	LEU	CD1-CG-CD2	-5.30	94.61	110.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4367	0	4476	132	1
2	B	1298	0	1280	39	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	259	0	279	13	0
4	A	1	0	0	0	0
5	A	43	0	30	1	0
6	A	65	0	62	9	0
7	B	2	0	0	0	0
8	A	2	0	0	1	0
All	All	6037	0	6127	171	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (171) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:HIS:NE2	1:A:237:TYR:HE2	0.93	1.41
1:A:233:HIS:NE2	1:A:237:TYR:CE2	1.79	1.24
1:A:233:HIS:CE1	1:A:237:TYR:HE2	1.81	0.97
1:A:233:HIS:CE1	1:A:237:TYR:CE2	2.54	0.95
2:B:26:LEU:O	2:B:30:ILE:HG13	1.69	0.93
2:B:101:ALA:O	2:B:103:ILE:HD12	1.75	0.87
1:A:449:ARG:HD2	1:A:450:ARG:HG3	1.60	0.81
1:A:368:SER:HB3	2:B:33:ILE:HD11	1.64	0.80
1:A:282:HIS:HA	1:A:285:PHE:CE1	2.16	0.80
1:A:106:MET:O	1:A:109:SER:OG	2.04	0.76
1:A:160:ILE:HD13	1:A:194:PHE:HB2	1.69	0.75
1:A:388:GLN:HE21	1:A:388:GLN:HA	1.50	0.74
1:A:364:ILE:O	1:A:368:SER:OG	2.06	0.74
1:A:233:HIS:NE2	1:A:237:TYR:CD2	2.55	0.74
6:A:801:HAS:ND	8:A:563:CMO:O	2.23	0.71
1:A:388:GLN:HA	1:A:388:GLN:NE2	2.06	0.71
2:B:5:HIS:C	2:B:7:ALA:H	1.95	0.70
1:A:236:VAL:HG12	1:A:239:TRP:CZ3	2.27	0.70
1:A:158:VAL:HG12	1:A:162:ILE:HD12	1.74	0.70
1:A:366:ASN:HB3	6:A:801:HAS:CMD	2.22	0.70
1:A:303:LEU:HB3	2:B:26:LEU:HG	1.73	0.69
1:A:230:TRP:O	1:A:230:TRP:CD1	2.46	0.68
1:A:156:THR:O	1:A:160:ILE:HG13	1.94	0.68
1:A:388:GLN:HE21	1:A:388:GLN:CA	2.06	0.68
1:A:105:LEU:C	1:A:162:ILE:HD11	2.14	0.67
1:A:48:ASN:ND2	1:A:454:ALA:HA	2.10	0.66
1:A:236:VAL:HB	6:A:801:HAS:C3C	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:ILE:HD13	6:A:801:HAS:H311	1.76	0.66
2:B:142:PRO:HA	2:B:166:VAL:CG2	2.27	0.65
3:C:13:LEU:O	3:C:14:VAL:C	2.35	0.65
2:B:18:TRP:CE3	3:C:12:ILE:HD12	2.32	0.64
2:B:34:ALA:O	2:B:37:LEU:HB2	1.97	0.64
1:A:382:PRO:HA	1:A:385:PHE:CZ	2.34	0.63
1:A:330:ARG:HB2	1:A:334:GLY:HA3	1.81	0.63
1:A:262:ASP:HB3	1:A:263:PRO:HD3	1.80	0.62
1:A:230:TRP:O	1:A:230:TRP:HD1	1.81	0.62
1:A:29:PHE:CE1	1:A:401:LEU:HD11	2.34	0.62
1:A:449:ARG:HH12	6:A:801:HAS:CGA	2.13	0.61
2:B:5:HIS:CE1	2:B:8:HIS:CD2	2.88	0.61
1:A:197:SER:O	1:A:201:VAL:HG23	2.00	0.61
1:A:29:PHE:CZ	1:A:401:LEU:HD11	2.36	0.61
1:A:122:LEU:HB2	1:A:123:PRO:HD3	1.82	0.60
1:A:367:ALA:HA	6:A:801:HAS:OMD	2.02	0.60
1:A:385:PHE:O	1:A:389:VAL:HG12	2.01	0.60
1:A:366:ASN:HB3	6:A:801:HAS:C2D	2.32	0.59
2:B:60:GLN:O	2:B:61:GLU:HB3	2.02	0.59
2:B:99:GLN:OE1	2:B:168:GLU:HG3	2.01	0.59
1:A:357:ILE:HB	1:A:358:PRO:HD3	1.85	0.59
1:A:233:HIS:O	1:A:236:VAL:HG22	2.03	0.58
2:B:5:HIS:CE1	2:B:8:HIS:HD2	2.22	0.58
1:A:339:LEU:HB3	1:A:340:PRO:HD2	1.86	0.58
1:A:230:TRP:C	1:A:230:TRP:CD1	2.77	0.58
1:A:262:ASP:HB2	1:A:511:VAL:HG11	1.86	0.58
1:A:370:THR:HB	3:C:30:PHE:CZ	2.39	0.57
1:A:241:LEU:HA	1:A:244:TYR:HB2	1.84	0.57
1:A:234:PRO:HG3	1:A:277:THR:HA	1.85	0.57
1:A:92:LEU:HB2	1:A:93:PRO:HD3	1.86	0.57
3:C:6:LYS:O	3:C:10:ALA:N	2.24	0.56
1:A:280:GLY:C	1:A:282:HIS:H	2.10	0.55
2:B:94:PRO:HB2	2:B:165:VAL:HG23	1.86	0.55
1:A:260:VAL:HB	2:B:11:ILE:HD13	1.88	0.55
2:B:141:ARG:O	2:B:145:TYR:OH	2.17	0.54
1:A:371:LEU:HG	3:C:26:VAL:HG12	1.90	0.54
1:A:498:LYS:HD2	1:A:500:GLU:HG2	1.90	0.54
1:A:18:LYS:HG2	1:A:408:LEU:HD23	1.89	0.53
1:A:498:LYS:HG3	1:A:501:LEU:H	1.74	0.53
1:A:254:GLN:O	1:A:340:PRO:HG3	2.09	0.53
1:A:388:GLN:CA	1:A:388:GLN:NE2	2.69	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:MET:HB3	1:A:155:SER:HB2	1.91	0.52
2:B:5:HIS:C	2:B:7:ALA:N	2.62	0.52
1:A:379:ALA:C	1:A:382:PRO:HD2	2.30	0.52
1:A:365:VAL:HG22	3:C:23:TRP:HA	1.92	0.52
1:A:119:VAL:O	1:A:123:PRO:HD3	2.11	0.51
1:A:326:LEU:C	1:A:328:GLY:H	2.13	0.51
1:A:229:TRP:HZ3	1:A:232:GLY:O	1.94	0.51
1:A:281:PHE:H	1:A:298:HIS:CD2	2.29	0.51
2:B:19:LEU:HA	2:B:22:SER:HB2	1.92	0.50
2:B:9:LYS:HE2	2:B:9:LYS:HA	1.92	0.50
1:A:304:PHE:O	1:A:307:VAL:HG23	2.12	0.50
1:A:86:GLN:HG2	1:A:159:SER:OG	2.11	0.50
1:A:285:PHE:CD2	1:A:369:PHE:CD2	2.99	0.50
1:A:406:PRO:HG3	1:A:413:ILE:HD12	1.94	0.50
1:A:262:ASP:HB2	1:A:511:VAL:CG1	2.42	0.49
1:A:409:THR:O	1:A:497:ARG:NH1	2.45	0.49
2:B:166:VAL:CG2	2:B:166:VAL:O	2.60	0.49
1:A:222:LEU:O	1:A:226:THR:OG1	2.26	0.49
1:A:153:VAL:O	1:A:156:THR:OG1	2.21	0.49
1:A:382:PRO:HA	1:A:385:PHE:CE2	2.48	0.49
1:A:434:ILE:HG22	1:A:473:ALA:HB2	1.93	0.49
1:A:515:PRO:O	1:A:517:ASP:N	2.46	0.49
1:A:466:PRO:HA	1:A:469:PHE:HD2	1.77	0.49
1:A:105:LEU:O	1:A:162:ILE:HD11	2.13	0.48
3:C:9:LEU:HA	3:C:12:ILE:HG12	1.95	0.48
2:B:125:VAL:HG21	2:B:133:SER:HB3	1.95	0.48
2:B:115:GLY:O	2:B:149:CYS:HA	2.13	0.48
1:A:346:PHE:O	1:A:349:PRO:HD2	2.13	0.48
1:A:398:MET:C	1:A:400:SER:H	2.17	0.48
3:C:20:LEU:O	3:C:21:VAL:C	2.52	0.48
1:A:498:LYS:HG2	1:A:501:LEU:HB3	1.95	0.47
2:B:40:HIS:CE1	2:B:41:THR:HG23	2.49	0.47
1:A:154:LEU:O	1:A:157:TRP:HB2	2.15	0.47
1:A:48:ASN:HD22	1:A:454:ALA:HA	1.78	0.47
1:A:294:TRP:CZ2	1:A:544:PRO:HG2	2.50	0.47
1:A:370:THR:HG21	2:B:36:THR:HB	1.97	0.47
2:B:83:VAL:HG12	2:B:84:LEU:N	2.29	0.46
1:A:134:THR:O	1:A:135:PHE:C	2.53	0.46
1:A:357:ILE:HG23	3:C:15:LEU:HD13	1.97	0.46
1:A:281:PHE:H	1:A:298:HIS:HD2	1.63	0.46
1:A:389:VAL:HG13	1:A:390:ALA:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:TRP:C	1:A:230:TRP:HD1	2.18	0.46
1:A:241:LEU:HD12	1:A:241:LEU:HA	1.78	0.46
1:A:280:GLY:C	1:A:282:HIS:N	2.70	0.46
1:A:126:ALA:O	1:A:128:GLU:HG2	2.16	0.46
2:B:166:VAL:HG23	2:B:166:VAL:O	2.16	0.45
1:A:76:ASN:HB3	5:A:800:HEM:CAC	2.47	0.45
1:A:435:MET:HG2	1:A:439:LEU:HD22	1.98	0.45
1:A:247:ILE:O	1:A:252:PRO:HD3	2.16	0.45
1:A:348:ALA:CB	1:A:399:GLY:HA3	2.46	0.45
1:A:188:VAL:HG21	1:A:269:PHE:HB3	1.99	0.45
1:A:235:ILE:O	1:A:238:PHE:HB3	2.16	0.45
1:A:185:MET:CE	1:A:265:ALA:HB1	2.47	0.45
2:B:97:VAL:O	2:B:166:VAL:HA	2.16	0.45
3:C:13:LEU:HD22	3:C:13:LEU:HA	1.49	0.45
1:A:345:ALA:HA	1:A:399:GLY:O	2.16	0.45
1:A:41:PHE:CE2	1:A:55:LEU:HB2	2.52	0.44
1:A:517:ASP:N	1:A:517:ASP:OD2	2.49	0.44
2:B:34:ALA:HA	2:B:37:LEU:HD22	1.98	0.44
2:B:23:LEU:O	2:B:24:ALA:C	2.51	0.44
1:A:308:PRO:O	1:A:311:MET:HB2	2.18	0.44
1:A:354:LEU:HA	1:A:357:ILE:HD12	1.99	0.44
1:A:371:LEU:HD11	3:C:27:TYR:HA	2.00	0.44
2:B:74:THR:HG21	2:B:80:THR:OG1	2.16	0.44
2:B:142:PRO:HA	2:B:166:VAL:HG21	1.99	0.44
1:A:329:GLY:C	1:A:330:ARG:HG3	2.38	0.44
1:A:450:ARG:O	2:B:157:HIS:CD2	2.70	0.44
1:A:170:TRP:CH2	1:A:180:PRO:HD3	2.53	0.44
1:A:280:GLY:HA3	1:A:542:TYR:OH	2.17	0.44
3:C:4:LYS:HE3	3:C:9:LEU:HD13	2.00	0.44
1:A:241:LEU:HG	1:A:269:PHE:CE2	2.52	0.44
1:A:41:PHE:CE1	1:A:55:LEU:HD13	2.52	0.44
1:A:174:ASN:HB3	1:A:177:LYS:HB2	2.01	0.43
1:A:67:GLN:HE22	1:A:127:ASN:H	1.66	0.43
2:B:146:ARG:HG2	2:B:147:ILE:N	2.34	0.43
1:A:324:GLY:HA3	1:A:335:TRP:HB2	2.01	0.43
1:A:264:MET:SD	2:B:15:GLU:HG2	2.59	0.42
1:A:388:GLN:HE21	1:A:388:GLN:N	2.17	0.42
1:A:445:LEU:O	1:A:446:ASN:HB2	2.19	0.42
1:A:389:VAL:HB	6:A:801:HAS:HBC2	2.01	0.42
1:A:369:PHE:O	1:A:370:THR:C	2.58	0.42
2:B:5:HIS:O	2:B:7:ALA:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:VAL:HG13	1:A:152:PHE:CZ	2.54	0.42
1:A:301:LEU:HA	1:A:304:PHE:HB2	2.01	0.42
1:A:370:THR:HG21	2:B:36:THR:CB	2.50	0.41
1:A:343:ASN:HA	1:A:344:PRO:HD2	1.96	0.41
1:A:363:GLY:HA2	1:A:366:ASN:HB2	2.01	0.41
1:A:339:LEU:HB3	1:A:340:PRO:CD	2.50	0.41
1:A:203:GLU:OE2	1:A:228:PHE:HB2	2.20	0.41
1:A:291:ASP:HA	1:A:292:PRO:HD2	1.83	0.41
2:B:74:THR:HG23	2:B:78:GLN:OE1	2.20	0.41
2:B:131:GLU:HG3	2:B:132:VAL:N	2.35	0.41
1:A:411:LYS:HG2	1:A:496:GLU:O	2.21	0.41
1:A:517:ASP:O	1:A:521:VAL:HB	2.21	0.41
1:A:119:VAL:O	1:A:123:PRO:CD	2.68	0.41
1:A:355:GLY:O	1:A:387:LEU:HB3	2.21	0.41
1:A:314:PHE:HB2	3:C:12:ILE:HG21	2.03	0.40
2:B:94:PRO:HB2	2:B:165:VAL:CG2	2.49	0.40
2:B:90:TYR:O	2:B:93:ASN:HB2	2.22	0.40
1:A:271:LEU:HA	1:A:271:LEU:HD23	1.83	0.40
1:A:335:TRP:O	1:A:339:LEU:HD22	2.21	0.40
1:A:449:ARG:NH1	6:A:801:HAS:CGA	2.82	0.40
1:A:79:VAL:HG21	1:A:117:LEU:HD13	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:GLU:OE1	2:B:166:VAL:N[4_545]	2.00	0.20

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	550/568 (97%)	470 (86%)	70 (13%)	10 (2%)	11 37
2	B	164/168 (98%)	135 (82%)	23 (14%)	6 (4%)	4 17
3	C	31/34 (91%)	12 (39%)	12 (39%)	7 (23%)	0 0
All	All	745/770 (97%)	617 (83%)	105 (14%)	23 (3%)	5 21

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	6	LYS
3	C	21	VAL
1	A	327	ARG
1	A	331	GLY
1	A	515	PRO
2	B	4	GLU
2	B	87	ALA
3	C	14	VAL
1	A	281	PHE
1	A	500	GLU
1	A	516	GLU
2	B	61	GLU
1	A	414	SER
2	B	46	PRO
3	C	23	TRP
3	C	28	ALA
3	C	5	PRO
3	C	20	LEU
1	A	104	GLY
1	A	334	GLY
3	C	19	ILE
1	A	499	PRO
2	B	123	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	448/462 (97%)	409 (91%)	39 (9%)	13 36
2	B	136/138 (99%)	122 (90%)	14 (10%)	9 26
3	C	26/27 (96%)	23 (88%)	3 (12%)	7 21
All	All	610/627 (97%)	554 (91%)	56 (9%)	11 33

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	GLU
1	A	30	LEU
1	A	48	ASN
1	A	56	LYS
1	A	82	GLN
1	A	89	MET
1	A	133	TYR
1	A	164	LEU
1	A	165	ASP
1	A	168	ARG
1	A	215	LEU
1	A	223	VAL
1	A	230	TRP
1	A	241	LEU
1	A	252	PRO
1	A	254	GLN
1	A	282	HIS
1	A	291	ASP
1	A	305	VAL
1	A	326	LEU
1	A	333	PHE
1	A	339	LEU
1	A	342	ASP
1	A	368	SER
1	A	369	PHE
1	A	388	GLN
1	A	430	LEU
1	A	434	ILE
1	A	439	LEU
1	A	449	ARG
1	A	478	LEU
1	A	486	TYR
1	A	497	ARG
1	A	498	LYS

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Mol	Chain	Res	Type
1	A	517	ASP
1	A	518	ARG
1	A	519	ARG
1	A	520	LEU
1	A	522	LEU
2	B	11	ILE
2	B	12	LEU
2	B	23	LEU
2	B	37	LEU
2	B	39	THR
2	B	61	GLU
2	B	72	VAL
2	B	77	ASN
2	B	91	GLN
2	B	99	GLN
2	B	111	ASP
2	B	125	VAL
2	B	159	ASN
2	B	166	VAL
3	C	13	LEU
3	C	15	LEU
3	C	18	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	48	ASN
1	A	63	GLN
1	A	76	ASN
1	A	254	GLN
1	A	298	HIS
1	A	388	GLN
1	A	446	ASN
2	B	5	HIS
2	B	8	HIS
2	B	69	GLN
2	B	73	GLN
2	B	117	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	CMO	A	563	4	0,1,1	0.00	-	0,0,0	0.00	-
5	HEM	A	800	1	30,50,50	2.03	9 (30%)	24,82,82	2.31	6 (25%)
6	HAS	A	801	1	45,72,72	2.07	8 (17%)	47,109,109	2.74	20 (42%)
7	CUA	B	802	2	0,1,1	0.00	-	0,0,0	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	CMO	A	563	4	-	0/0/0/0	0/0/0/0
5	HEM	A	800	1	-	0/10/54/54	0/0/8/8
6	HAS	A	801	1	-	0/30/82/82	0/0/8/8
7	CUA	B	802	2	-	0/0/0/0	0/0/0/0

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	800	HEM	C3B-C4B	-6.56	1.46	1.51
6	A	801	HAS	C4C-NC	-5.58	1.29	1.36
5	A	800	HEM	C3D-C4D	-4.24	1.46	1.51
5	A	800	HEM	C2C-C1C	-2.79	1.47	1.52
5	A	800	HEM	C2D-C1D	-2.39	1.44	1.51
5	A	800	HEM	C3C-CAC	2.07	1.55	1.51
5	A	800	HEM	FE-NB	2.30	2.09	1.97
5	A	800	HEM	C1C-NC	2.58	1.39	1.36
5	A	800	HEM	C4C-NC	2.77	1.39	1.36
5	A	800	HEM	FE-NC	2.99	2.07	1.95
6	A	801	HAS	C2A-C3A	3.00	1.46	1.37
6	A	801	HAS	C3C-CAC	3.18	1.54	1.47
6	A	801	HAS	C1D-CHB	3.64	1.49	1.39
6	A	801	HAS	C1A-CHA	3.69	1.50	1.39
6	A	801	HAS	C1C-CHC	3.88	1.50	1.39
6	A	801	HAS	C2D-C3D	4.83	1.46	1.40
6	A	801	HAS	C3C-C2C	7.38	1.50	1.40

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	801	HAS	CMC-C2C-C3C	-10.32	104.90	125.09
6	A	801	HAS	CMC-C2C-C1C	-7.42	116.09	128.36
5	A	800	HEM	C3B-CAB-CBB	-5.04	116.73	124.46
6	A	801	HAS	CAD-CBD-CGD	-4.47	104.55	112.75
6	A	801	HAS	C13-C12-C11	-3.59	109.74	114.51
6	A	801	HAS	CBA-CAA-C2A	-3.51	106.24	112.53
6	A	801	HAS	C21-C22-C23	-3.48	120.20	127.76
6	A	801	HAS	C25-C23-C22	-2.69	118.22	123.50
6	A	801	HAS	C3C-CAC-CBC	-2.63	120.93	126.32
6	A	801	HAS	CAA-CBA-CGA	-2.60	107.99	112.75
6	A	801	HAS	C4D-C3D-C2D	-2.53	104.54	107.07
6	A	801	HAS	C13-C14-C15	-2.40	122.54	127.76
6	A	801	HAS	C17-C18-C19	-2.24	122.89	127.76
6	A	801	HAS	OMD-CMD-C2D	-2.02	121.02	125.11
6	A	801	HAS	CBD-CAD-C3D	2.11	116.31	112.53
6	A	801	HAS	CMA-C3A-C2A	2.30	130.05	125.24
6	A	801	HAS	C27-C19-C20	2.66	119.47	115.41
6	A	801	HAS	C26-C15-C16	2.77	119.63	115.41
6	A	801	HAS	C3C-C4C-NC	2.88	116.39	110.94
5	A	800	HEM	CMB-C2B-C3B	3.04	124.12	116.53
6	A	801	HAS	CAD-C3D-C4D	3.11	130.38	127.01
5	A	800	HEM	CMD-C2D-C3D	3.53	129.97	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	800	HEM	CMC-C2C-C3C	3.77	125.95	116.53
5	A	800	HEM	CAD-C3D-C4D	4.41	128.04	112.47
6	A	801	HAS	C25-C23-C24	4.56	122.37	115.41
5	A	800	HEM	CAD-C3D-C2D	5.17	128.07	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	563	CMO	1	0
5	A	800	HEM	1	0
6	A	801	HAS	9	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	552/568 (97%)	0.19	45 (8%) 14 9	33, 43, 49, 58	0
2	B	166/168 (98%)	0.34	19 (11%) 7 4	37, 44, 48, 52	0
3	C	33/34 (97%)	0.19	4 (12%) 6 3	45, 56, 74, 92	0
All	All	751/770 (97%)	0.22	68 (9%) 11 7	33, 43, 51, 92	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	12	TYR	9.7
1	A	14	ALA	9.2
1	A	11	VAL	7.9
1	A	13	GLU	7.1
1	A	502	ALA	7.0
1	A	503	GLU	6.3
1	A	501	LEU	6.1
3	C	2	GLU	5.9
2	B	168	GLU	5.7
1	A	495	ARG	5.2
1	A	342	ASP	4.7
1	A	493	LEU	4.6
1	A	416	ALA	4.5
1	A	504	ALA	4.4
2	B	7	ALA	4.3
2	B	60	GLN	4.2
1	A	514	GLY	4.2
1	A	499	PRO	4.1
2	B	39	THR	4.1
1	A	415	ASP	4.0
3	C	3	GLU	4.0
2	B	6	LYS	4.0
1	A	497	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	498	LYS	3.7
1	A	414	SER	3.6
1	A	552	HIS	3.6
3	C	34	GLY	3.4
1	A	458	ASP	3.4
2	B	144	GLU	3.4
1	A	330	ARG	3.4
1	A	418	ARG	3.3
2	B	76	PRO	3.3
2	B	82	TYR	3.2
1	A	513	SER	3.0
3	C	4	LYS	3.0
2	B	38	ALA	3.0
1	A	518	ARG	2.9
1	A	494	SER	2.9
1	A	317	ALA	2.9
2	B	40	HIS	2.8
1	A	319	SER	2.8
2	B	13	ALA	2.7
2	B	20	ALA	2.7
1	A	368	SER	2.6
1	A	327	ARG	2.6
1	A	419	ARG	2.6
1	A	455	GLN	2.5
1	A	215	LEU	2.5
2	B	107	ILE	2.5
1	A	402	TYR	2.5
1	A	63	GLN	2.5
2	B	159	ASN	2.5
2	B	83	VAL	2.4
1	A	522	LEU	2.4
1	A	105	LEU	2.4
1	A	293	THR	2.4
1	A	526	ARG	2.3
1	A	496	GLU	2.3
1	A	452	TYR	2.2
2	B	102	GLU	2.2
2	B	79	TYR	2.2
2	B	61	GLU	2.2
1	A	54	LEU	2.2
1	A	315	THR	2.1
1	A	517	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	332	LEU	2.1
2	B	108	THR	2.0
1	A	457	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	HEM	A	800	43/43	0.97	0.18	0.08	39,44,46,48	0
6	HAS	A	801	65/65	0.95	0.16	-0.26	26,43,46,47	0
7	CUA	B	802	2/2	0.99	0.10	-1.06	44,44,44,47	0
8	CMO	A	563	2/2	0.99	0.23	-	81,81,81,85	0
4	CU1	A	803	1/1	0.99	0.04	-	46,46,46,46	0

6.5 Other polymers (i)

There are no such residues in this entry.